Table 2. *Main M–X and X–X distances* (Å) *in UZr_6FO_{14} (e.s.d.'s in parentheses)*

Symmetry operators: (i) $-\tfrac{1}{2} + x,y$, $\tfrac{1}{2} - z$; (ii) $\tfrac{1}{2} + x,y$, $\tfrac{1}{2} - z$; (iii) $1 - x$, $1 - y$, $- z$; (iv) x,y, $- 1 + z$; (v) x,y, $1 + z$; (vi) x, $\tfrac{1}{2} - y,z$; (vii) $\tfrac{1}{2} - x$, $1 - y$, $-\tfrac{1}{2} + z$.

$M(1)-X(2^i)$	2·09 (2)		
$X(1^i)$	2·11 (2)	$X(7)-X(7^{vi})$	2·54 (4)
$X(1^{iii})$	2·12 (2)	$X(1)-X(1^{iii})$	2·55 (4)
$X(2^{iv})$	2·17 (2)	$X(3^v)-X(2)$	2·55 (2)
$X(3)$	2·17 (2)	$X(5)-X(7)$	2·55 (3)
$X(1)$	2·19 (2)	$X(4)-X(5^v)$	2·58 (3)
$X(3^i)$	2·40 (2)	$X(3)-X(1)$	2·59 (3)
$X(1^{vii})$	2·93 (2)	$X(7^v)-X(6)$	2·59 (2)
		$X(5)-X(3)$	2·61 (3)
$M(2)-X(4^{ii})$	2·05 (2)	$X(6)-X(8)$	2·62 (2)
$X(2^{iv})$	2·14 (2)	$X(8^{ii})-X(6^{iv})$	2·64 (2)
$X(3^{ii})$	2·15 (2)	$X(1)-X(1^i)$	2·66 (3)
$X(4^{iv})$	2·16 (2)	$X(4)-X(6)$	2·68 (3)
$X(5)$	2·22 (2)	$X(3)-X(3^i)$	2·68 (2)
$X(5^{ii})$	2·26 (2)	$X(7)-X(8)$	2·70 (3)
$X(3)$	2·28 (2)	$X(2^{iv})-X(1^{iii})$	2·70 (3)
$X(2^{ii})$	3·15 (2)	$X(5)-X(5^i)$	2·71 (2)
		$X(7)-X(7^i)$	2·72 (2)

Table 2 (*cont.*)

$M(3)-X(6^i)$	2·03 (2)	$X(2^i)-X(2^{iv})$	2·72 (2)
$X(6^{iv})$	2·10 (2)	$X(2)-X(4)$	2·73 (3)
$X(5^i)$	2·15 (2)	$X(4^i)-X(6^{iv})$	2·76 (3)
$X(4^{iv})$	2·19 (2)	$X(4^{iv})-X(4^{ii})$	2·78 (1)
$X(7^i)$	2·20 (2)	$X(2)-X(3)$	2·78 (2)
$X(7)$	2·22 (2)	$X(1^i)-X(1^{vii})$	2·82 (4)
$X(5)$	2·28 (2)	$X(6^{iv})-X(6^i)$	2·83 (1)
$X(8^{iv})$	2·68 (1)	$X(8^{iv})-X(8^i)$	2·88 (2)
		$X(5)-X(6)$	2·92 (3)
$M(4)-X(8^{ii})$	2·03 (3)	$X(2^{iv})-X(4^{ii})$	2·93 (3)
$X(8^{iv})$	2·09 (3)	$X(1^{iii})-X(2^i)$	3·00 (3)
$X(7^{ii})$	2 × 2·16 (2)		
$X(7)$	2 × 2·26 (2)		
$X(6^{iv})$	2 × 2·35 (2)		

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Single-Crystal Structure of Copper Lanthanum Telluride $Cu_{0.28}LaTe_2$: A Disordered Tunnel Structure

By Nguyen-Huy Dung, Marie-Paule Pardo and Pierre Boy

Laboratoire de Physique (Laboratoire de Chimie Minérale Structurale, associé au CNRS n° 200), Faculté des Sciences Pharmaceutiques et Biologiques de Paris V, 4 avenue de l'Observatoire, 75270 Paris CEDEX 06, France

Abstract. $M_r = 411·90$, orthorhombic, *Pbcm*, $a = 7·726$ (4), $b = 8·603$ (5), $c = 6·246$ (2) Å, $D_x = 6·59$ Mg m^{-3}, $Z = 4$, $F(000) = 676$, $T = 298$ K. The structure has been refined by the least-squares method to a final R value of 0·05 for 622 independent reflections. The eightfold-coordinated La atom is inside a bicapped triangular prism of Te atoms. The polyhedra are connected so that they create pentagonal tunnels in the [001] direction which are occupied by Cu atoms in positional disorder. The Cu atoms are placed in partially occupied Cu sites, and these sites form a zigzag chain, parallel to the c axis.

Introduction. In previous investigations, Pardo & Flahaut (1971) described the ternary phase diagram Cu–La–Te, especially the quasi-binary system $Cu_2Te–La_2Te_3$. In order to complete the phase diagram, we are studying the system $Cu–LaTe_2$ (a homogeneity domain is found between $LaTe_2$ and $SmTe_2$ which exists from lanthanum to samarium). These phases are obtained by mixing Cu, La and Te elements (or Cu and $LaTe_2$) in appropriate proportions, and heating them in evacuated silica ampoules at 1178 K for one day, and annealing at 678 K for two days.

Experimental. Prepared from the elements using the iodine vapour transport technique at 1275 K; microprobe analysis confirmed absence of iodine and the chemical formula obtained after refinement; parallelepiped crystal (500 × 200 × 100 μm); systematic absences ($0kl$, $k = 2n + 1$; $h0l$, $l = 2n + 1$) led to the space groups *Pbcm* or $Pbc2_1$; Syntex $P2_1$ diffractometer, ω–2θ scan technique, graphite-monochromated Mo $K\alpha$ radiation, $\sin\theta/\lambda$ range 0·02 to 0·7 Å^{-1}; 819 intensities collected and corrected for Lorentz, polarization and absorption effects with the crystal shape approximated by a sphere ($\mu = 25·9$ mm^{-1}); heavy-atom method. The presence of very important peaks on [001] in the Patterson function $P(u,v,w)$ shows the existence of a mirror normal to this axis. Hence the non-centrosymmetric space group $Pbc2_1$ was rejected. Scattering factors and anomalous-dispersion corrections from *International Tables for X-ray Crystallography* (1974). In the first stage of the refinement, an average atom was used because the scattering factors for La and Te atoms are very close. In the second stage, they could be distinguished completely by their individual thermal factors and their surroundings.

The Cu atom in positional disorder on the 8(e) site was located on difference $(F_o - F_c)$ Fourier maps. The positional, occupancy and anisotropic thermal parameters were refined by the full-matrix least-squares method, minimizing $\sum w(\Delta F)^2$, with ORXFLS (Busing, 1971) using 622 reflections with $I > 3\sigma(I)$. $R = 0.05$, $R_w = 0.07$ (positional coordinates, occupancies and anisotropic thermal parameters varied simultaneously during the refinement); $w_F = 1/\sigma_F^2 = I/\sigma^2(I)$.

Discussion. Positional parameters are listed in Table 1.*
The eightfold-coordinated La atom is inside a bicapped triangular prism of Te atoms with two distances shorter than the remaining six (Fig. 1). These distances are close to those observed in the LaTe$_2$ structure (Pardo, Flahaut & Domange 1964; Wang, Steinfink & Bradley 1966).

Those polyhedra which are related by an inversion centre share a common edge; those related by a c glide plane alternately share a common edge or a vertex; those related by a b glide plane have only a common edge. If we consider a series of four bicapped triangular prisms around the La atom, these types of connection create a pentagonal tunnel of Te atoms which surrounds a band of Cu sites themselves forming a zigzag chain (Fig. 2). Two types of Cu—Cu distance are observed. The first is very short (1.27 Å) and is related to a pair of sites which cannot be occupied simultaneously. The second is longer and corresponds to the distance between two neighbouring pairs. These sites form a zigzag chain parallel to the c axis and are occupied by Cu atoms in a disordered way. The disorder may be static (the Cu atoms inside such sites may occupy one of the vacancies) or dynamic (the Cu atom may oscillate from one site to the next).

The Cu—Cu distances are in good agreement with those observed in Cu$_{2-x}$Mo$_3$S$_4$ compounds (Yvon, Paoli, Flükiger & Chevrel, 1977).

The Cu sites are inside pentagonal tunnels of the Te atoms previously described. The tunnels share one common face. The Cu atom is fourfold coordinated to the Te atoms, and two adjacent tetrahedra around one pair share a common face, while, from one pair to another, two tetrahedra share only one edge (Fig. 3).

The Cu—Te distances are comparable to those observed in CuTe (Baranova 1964) or in non-stoichiometric phases: the so-called hexagonal β_1-Cu$_7$Te$_4$ (Baranova, 1967) or β_2-Cu$_{2-x}$Te (Baranova, 1969) and tetragonal γ_1- or γ_2-Cu$_{4-x}$Te$_2$ phases (Baranova & Pinsker, 1969) with statistical disorder of Cu atoms on their sites.

The second main feature in this structure is the presence of Te(2) atom pairs which are covalently

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38385 (6 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Positional* ($\times 10^4$), *occupational and equivalent isotropic thermal* (Å^2) *parameters with e.s.d.'s in parentheses*

$$B_{eq} = \tfrac{4}{3}\sum_i\sum_j\beta_{ij}\mathbf{a}_i\cdot\mathbf{a}_j$$

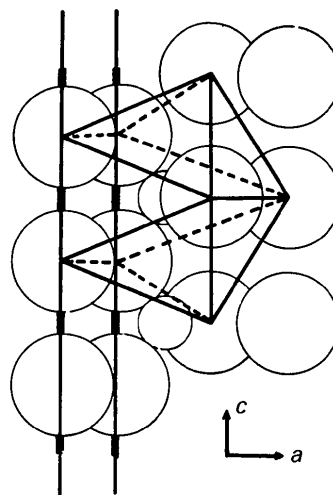|	x	y	z	Occupancy	$B_{eq}(\text{Å}^2)$
La	2403 (1)	4411 (1)	$\tfrac{1}{4}$	1	1.00 (2)
Te(1)	3823 (2)	926 (1)	$\tfrac{1}{4}$	1	0.91 (2)
Te(2)	9186 (1)	$\tfrac{1}{4}$	0	1	1.04 (2)
Cu	5920 (14)	2979 (15)	770 (25)	0.28 (1)	1.83 (3)

Fig. 1. One Te-atom polyhedron around an La atom. The Te chain axis is shown by a heavy line. Increased circle size represents La and Te atoms respectively.
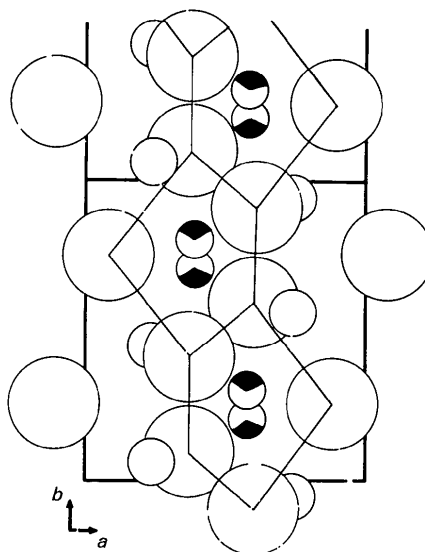

Fig. 2. Projection of the structure on to (001). Diagram of a tellurium pentagonal tunnel sequence enclosing a pair of copper sites in positional disorder. Increased circle size represents Cu, La and Te atoms respectively.
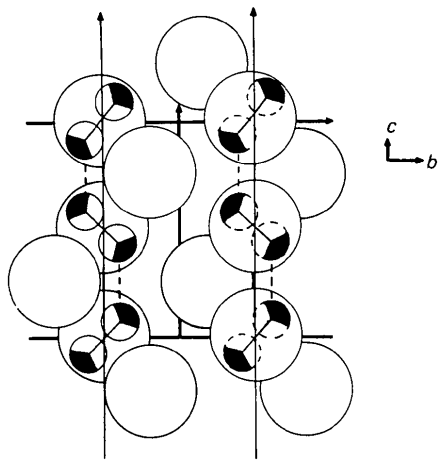
Fig. 3. Diagram of the tetrahedral surroundings of Cu atom chains. La atoms are omitted. The two types of distance are shown schematically (the dotted line represents the long distance, and the solid line the short distance).

bonded at a distance of 3.123 (1) Å, as found in the $LaTe_2$ structure. These Te(2) atoms do not form a plane as in $LaTe_2$, but only chains parallel to the c axis. The Te(2) atoms are linked to four La atoms and to two partially occupied sites of Cu atoms (2.60 Å), while the Te(1) atoms are also connected to four La atoms and to six partially occupied Cu sites (from 2.63 to 2.76 Å). Table 2 summarizes some interatomic distances.

We may expect the homogeneity range to be directly correlated with the Cu atom concentration as seen in lattice-parameter variations from $Cu_{0.28}LaTe_2$ to $Cu_{0.50}LaTe_2$, but further investigations are needed. Moreover, although the +I oxidation state of the Cu atoms is not clearly established, we can suggest an ionocovalent bonding model where Te atoms may exhibit a certain metallic character, as currently observed in binary metallic telluride compounds. There is no direct bonding between La and Cu atoms. Electrical properties will be investigated with respect to the crystal structure analysis.

Table 2. *Interatomic distances* (Å) *with e.s.d.'s in parentheses*

Symmetry code

(i) $1-x,y,z$;	(v) $x,\frac{1}{2}-y,-z$;
(ii) $2+x,y,z$;	(vi) $1-x,-\frac{1}{2}+y,z$;
(iii) $1-x,1-y,-z$;	(vii) $1-x,\frac{1}{2}+y,z$
(iv) $x,y,\frac{1}{2}-z$;	

La—Te(1)	3.192 (2)	Te(2)—Cu	2×2.60 (1)
La—Te(1^{vii})	3.194 (2)	Te(2)—La^{iii}	2×3.318 (2)
La—Te(2^{iii})	2×3.318 (2)	Te(2)—La^{ii}	2×3.364 (2)
La—Te(1^{v})	2×3.323 (1)	Te(2)—Te(2)	2×3.123 (1)
La—Te(2^{i})	2×3.364 (2)		
Te(1)—Cu	2×2.63 (1)	Cu—Te(2)	2.60 (1)
Te(1)—Cu^{vi}	2×2.76 (1)	Cu—Te(1)	2.63 (1)
Te(1)—Cu^{v}	2×2.77 (1)	Cu—Te(1^{vii})	2.76 (1)
Te(1)—La^{vi}	2×3.192 (2)	Cu—Te(1^{v})	2.77 (1)
Te(1)—La^{vi}	2×3.194 (2)	Cu—Cu^{v}	1.27 (3)
Te(1)—La^{v}	2×3.323 (1)	Cu—Cu^{iv}	2.16 (3)

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Polymorphisme de $LaYbS_3$. Affinement des Structures des Deux Variétés

PAR N. RODIER ET R. JULIEN

Laboratoire de Chimie Minérale, Faculté des Sciences Pharmaceutiques et Biologiques, rue J.-B. Clément, 92290 Chatenay-Malabry, France

ET VOVAN TIEN

Laboratoire de Chimie Minérale Structurale, associé au CNRS n° 200, Faculté des Sciences Pharmaceutiques et Biologiques, 4 avenue de l'Observatoire, 75270 Paris CEDEX 06, France

Abstract. Low-temperature variety, $M_r = 408.1$, orthorhombic, $B22_12$, $a = 12.604$ (5), $b = 9.493$ (5), $c = 3.914$ (3) Å, $D_x = 5.79$ Mg m^{-3}, $Z = 4$; $F(000) = 700$; isostructural with $NdYbS_3$. High-temperature variety, $M_r = 408.1$, orthorhombic, *Pnam*, $a = 7.357$ (4), $b = 6.698$ (4), $c = 9.867$ (5) Å, $D_x = 5.57$ Mg m^{-3}, $Z = 4$; $F(000) = 700$; isostructural with $YScS_3$. The two structures were refined to $R = 0.027$,